Predicted Bioaccumulation factor for 1897-45-6 from Consensus method

Prediction results

Endpoint	Experimental value (CAS= 1897-45-6) Sources: Dimetrov 2005, Arnot 2006, and Zhao 2008	Predicted value[a]
Bioaccumulation factor Log10	1.25	1.65
Bioaccumulation factor	17.82	44.20

[a]Note: the test chemical was present in the external test set.

Individual Predictions

Method	Predicted value Log10
Hierarchical clustering	1.81
Single model	2.22
Group contribution	2.00
Nearest neighbor	0.54

Test chemical

Predictions for the test chemical and for the most similar chemicals in the external test set

Note: No chemicals in the test set exceed a minimum similarity coefficient of 0.5 for comparison purposes

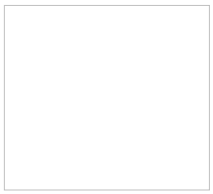
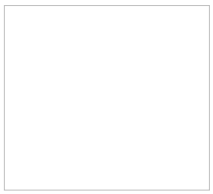
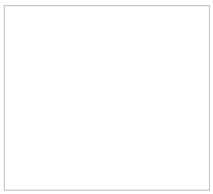
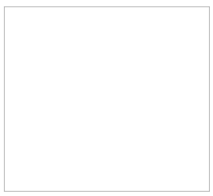
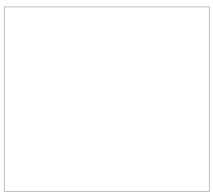
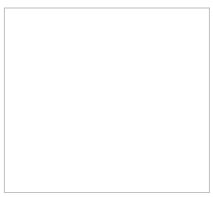
Predictions for the test chemical and for the most similar chemicals in the training set

If the predicted value matches the experimental values for similar chemicals in the training set (and the similar chemicals were predicted well), one has greater confidence in the predicted value.

Chemicals	MAE*
Entire set	0.42
Similarity coefficient ≥ 0.5	0.32

*Mean absolute error in Log10

CAS	Structure	Similarity	Experimental value	Predicted value

1897-45-6 (test chemical)			1.25	1.65
91-15-6		0.84	0.40	0.58
626-17-5		0.77	0.40	0.63
1689-84-5		0.70	0.83	1.36
623-26-7		0.69	0.16	0.63
767-00-0		0.58	0.91	0.70